Two-stage subspace identification for softsensor design and disturbance estimation

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Abstract

Softsensors or virtual sensors are key technologies in industry because important variables such as product quality are not always measured on-line. In the present work, two-stage subspace identification (SSID) is proposed to develop highly accurate softsensors that can take into account the influence of unmeasured disturbances on estimated key variables explicitly. The proposed two-stage SSID method can estimate unmeasured disturbances without the assumptions that the conventional Kalman filtering technique must make. Therefore, it can outperform the Kalman filtering technique when innovations are not Gaussian white noises or the characteristics of disturbances do not stay constant with time. The superiority of the proposed method over the conventional methods is demonstrated through numerical examples and application to an industrial ethylene fractionator.

Key words: Softsensor, Subspace identification, Disturbance estimation, Modeling

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1 Introduction

Product quality is not always measured on-line and its estimates are useful for realizing feedback control; thus softsensors play an important role in achieving better industrial productivity. To build softsensors, statistical methods or data-driven approaches have been widely used although physical model-based approaches are preferrable in principle. A research trend in the field of data-driven softsensor design was briefly surveyed by Kano and Nakagawa [1]. They showed that artificial neural network (ANN) had been dominant in the literature since the middle 90's, while partial least squares (PLS) regression was popular in industry. As for nonlinear methods, support vector machine (SVM) and support vector regression (SVR) have attracted researchers' and engineers' attention in the last few years. Another method for developing softsensors is subspace identification (SSID), which can build a state space model from input-output data. SSID is a useful tool to build a dynamic inferential model of a multivariable process, but SSID-based softsensor design seems to have received relatively little attention so far.

PLS-based softsensors have been investigated by many researchers since early 90's [2,3]. They are very popular in industry because of the simplicity and ability to cope with a collinearity problem. When many process variables are used as input variables of a statistical model, the highly correlated nature of process data must be taken into account. Kano et al. [4] investigated PLS-based inferential models, compared steady-state, static, and dynamic inferential models, and found that the estimation accuracy could be greatly improved by using dynamic models. More recently, Lin et al. [5] implemented a dynamic PLS model to a cement kiln system for providing smoother estimation than a static regression model. PLS has been applied not only to continuous processes but also batch processes, in which process dynamics are often modeled via multiway PLS [6] that is similar to dynamic PLS for continuous processes. Flores-Cerrillo and MacGregor [7] investigated adaptive PLS to update models from batch to batch. They also proposed an inferential strategy for controlling end-product quality properties of a batch process by adjusting the complete trajectories of the manipulated variables [8]. Aguado et al. [9] compared principal component regression (PCR), PLS, and ANN for nutrient estimation in a sequencing batch reactor (SBR) and showed that batch-wise unfolding PLS models outperformed the other approaches. Another extension of PLS to cope with multirate dynamic systems was proposed by Lu et al. [10]. In addition, recursive PLS has been investigated because the maintenance of inferential models is crucial from the practical viewpoint [11,12]. Another important issue in practice is to check the reliability of prediction. Kamohara et al. [13] investigated the integration of a dynamic PLS-based softsensor with multivariate statistical process control (MSPC) to check the reliability of both the softsensor and an analyzer.

As mentioned above, PLS has been widely accepted as a useful technique for softsensor design. However, it might not be the best approach for modeling dynamics of multivariable processes. Amirthalingam and Lee [14] investigated SSID to develop an inferential control model for a continuous pulp digester, because the state estimation-based approach is preferred to the output estimation-based approach if a dynamic estimator for a multivariable process is to be designed. Amirthalingam et al. [15] developed a two-step procedure to build SSID-based inferential control models, in which the stochastic part was idetified from historical data and the deterministic part was identified from plant test data. Similar to dynamic PLS, SSID is also used for modeling batch processes [16,17]. Although SSID is useful for modeling maltivariable processes, the performance of the conventional softsensor design method based on SSID and Kalman filter is limited due to the assumption that innovations are Gaussian white noises and the characteristics of disturbances stay constant with time. In other words, the conventional method does not use measured variables effectively, while measured variables contain valuable information on the process including unmeasured disturbances that have serious influence on key variables.

In the present work, two-stage SSID is proposed to develop highly accurate softsensors that can take into account the influence of unmeasured disturbances on key variables explicitly. The proposed method can estimate unmeasured disturbances without assumptions that the conventional Kalman filtering technique must make. The usefulness of the proposed method is demonstrated through numerical examples and their application to an industrial ethylene fractionator.

The remainder of this paper is organized as follows. In section 2, a conventional softsensor design method is explained in brief. In section 3, the proposed two-stage SSID method is described in detail. Validation results are provided in sections 4 and 5, where the conventional methods and the proposed two-stage SSID method are compared in prediction performance. Finally, conclusions are given in section 6.

2 Conventional SSID-based Method

In this section, a conventional softsensor design method based on SSID is briefly explained.

2.1 Subspace Identification

SSID is a method for identifying the following state space model directly from input-output data by using QR decomposition and singular value decomposition (SVD) [18].

$$\boldsymbol{x}(t+1) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{K}\boldsymbol{e}(t) \tag{1}$$

$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t) + \boldsymbol{D}\boldsymbol{u}(t) + \boldsymbol{e}(t) \tag{2}$$

where, $\boldsymbol{x}$, $\boldsymbol{u}$, $\boldsymbol{y}$, and $\boldsymbol{e}$ denote state, input, output, and innovation vectors, respectively, and $\boldsymbol{K}$ is the Kalman gain.

Although various algorithms for SSID have been proposed and they use different algorithms for estimating coefficient matrices, all algorithms adopt fundamentally the same approach: derive a subspace spanned by state variables from a part of input-output data, and then estimate coefficient matrices by using the derived subspace from the other part of input-output data.

2.2 Conventional SSID-based Method

In the conventional SSID-based softsensor design method, a state space model is identified through SSID, state variables are estimated with the Kalman filtering technique, and finally key variables such as product quality are estimated [14].

To build a softsensor, state variables $\boldsymbol{x}$ need to be estimated from measured output variables $\boldsymbol{y}_m$ and measured input variables $\boldsymbol{u}$, because key variables $\boldsymbol{y}_q$ are not measured on-line. The process model is given by:

$$\boldsymbol{x}(t+1) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{K}_m\boldsymbol{e}_m(t) \tag{3}$$

$$\begin{bmatrix} \boldsymbol{y}_q(t) \\ \boldsymbol{y}_m(t) \end{bmatrix} = \begin{bmatrix} \boldsymbol{C}_q \\ \boldsymbol{C}_m \end{bmatrix} \boldsymbol{x}(t) + \begin{bmatrix} \boldsymbol{D}_q \\ \boldsymbol{D}_m \end{bmatrix} \boldsymbol{u}(t) + \begin{bmatrix} \boldsymbol{e}_q(t) \\ \boldsymbol{e}_m(t) \end{bmatrix} \tag{4}$$

On the basis of this model, estimates of state variables $\hat{\boldsymbol{x}}$ are derived through the following filtering equations:

$$\hat{\boldsymbol{x}}(t+1 \mid t) = \boldsymbol{A}\hat{\boldsymbol{x}}(t \mid t) + \boldsymbol{B}\boldsymbol{u}(t) \tag{5}$$

$$\begin{aligned} \hat{\boldsymbol{x}}(t \mid t) &= \hat{\boldsymbol{x}}(t \mid t-1) \\ &\quad + \boldsymbol{K}_m \left\{ \boldsymbol{y}_m(t) - \boldsymbol{C}_m\hat{\boldsymbol{x}}(t \mid t-1) - \boldsymbol{D}_m\boldsymbol{u}(t) \right\} \end{aligned} \tag{6}$$

where $\hat{\boldsymbol{x}}(t+i \mid t)$ denotes i step ahead prediction of $\boldsymbol{x}$ on data up to time t. Finally, $\boldsymbol{y}_q$ is estimated.

$$\hat{\boldsymbol{y}}_q(t) = \boldsymbol{C}_q\hat{\boldsymbol{x}}(t \mid t) + \boldsymbol{D}_q\boldsymbol{u}(t) \tag{7}$$

Stochastic effects including disturbances and noises can be taken into account with the Kalman filter. For the effective functioning of the Kalman filter, disturbances should be generated from Gaussian white noises, and dynamics from the white noises to the output variables should stay constant with time. However, in actual processes, such assumptions are not always valid.

3 Two-Stage Subspace Identification

The procedure for two-stage SSID is as follows: 1) identify a state space model by using measured input and output variables, 2) estimate unmeasured disturbance variables from residual variables, and 3) identify a state space model to estimate key variables from the estimated disturbance variables and the other measured input variables.

It is assumed that a process is described by a linear state space model of the form:

$$\boldsymbol{x}(t+1) = \boldsymbol{A}_{real}\boldsymbol{x}(t) + \boldsymbol{B}_{real}\begin{bmatrix}\boldsymbol{u}_d(t)\\ \boldsymbol{u}_s(t)\end{bmatrix} + \boldsymbol{w}(t) \tag{8}$$

$$\begin{bmatrix}\boldsymbol{y}_q(t)\\ \boldsymbol{y}_m(t)\end{bmatrix} = \boldsymbol{C}_{real}\boldsymbol{x}(t) + \boldsymbol{D}_{real}\begin{bmatrix}\boldsymbol{u}_d(t)\\ \boldsymbol{u}_s(t)\end{bmatrix} + \boldsymbol{v}(t) \tag{9}$$

where $\boldsymbol{u}_d \in \Re^d, \boldsymbol{u}_s \in \Re^s, \boldsymbol{y}_q \in \Re^q, \boldsymbol{y}_m \in \Re^m$ are measured input variables, unmeasured disturbance variables, quality variables to be estimated, and measured output variables, respectively. In addition, $\boldsymbol{w} \in \Re^n$ and $\boldsymbol{v} \in \Re^{q+m}$ are white noises. Unmeasured disturbance variables $\boldsymbol{u}_s$ and noises $\boldsymbol{w}, \boldsymbol{v}$ have common characteristics with respect to being unmeasured, but $\boldsymbol{u}_s$ are not limited to white noises.

3.1 Identification (1st stage)

First, a state space model from measured input variables $\boldsymbol{u}_d$ to measured output variables $\boldsymbol{y}_m$ is identified through SSID.

$$\boldsymbol{x}_1(t+1) = \boldsymbol{A}_1\boldsymbol{x}_1(t) + \boldsymbol{B}_1\boldsymbol{u}_d(t) \tag{10}$$

$$\boldsymbol{y}_m(t) = \boldsymbol{C}_1\boldsymbol{x}_1(t) \tag{11}$$

where the subscript 1 denotes the 1st stage of identification. At this stage, it is assumed that $\boldsymbol{u}_d$ satisfy the persistently exciting condition.

3.2 Estimation of disturbance variables

The influence of the measured input variables $\boldsymbol{u}_d$ on the measured output variables $\boldsymbol{y}_m$ was modeled in the previous step. However, there must be residuals because $\boldsymbol{y}_m$ are affected not only by the measured input variables but also by unmeasured factors including $\boldsymbol{u}_s$. In other words, residual variables $\Delta\boldsymbol{y}_m$ defined as

$$\Delta\boldsymbol{y}_m = \boldsymbol{y}_m - \hat{\boldsymbol{y}}_m \tag{12}$$

have valuable information about the unmeasured disturbance variables $\boldsymbol{u}_s$. To estimate $\boldsymbol{y}_q$ with accuracy, it is worth estimating $\boldsymbol{u}_s$ from $\Delta\boldsymbol{y}_m$ and using the estimated disturbances $\hat{\boldsymbol{u}}_s$ as input variables together with $\boldsymbol{u}_d$. However, it is possible that the residual variables $\Delta\boldsymbol{y}_m$ are linearly dependent and not persistently exciting. Therefore, it is necessary to derive $\hat{\boldsymbol{u}}_s$ that satisfy the persistently exciting condition.

The first step to estimate $\boldsymbol{u}_s$ is to define block Hankel matrices $\boldsymbol{U}_{1|k,s} \in \Re^{ks\times N}$

and $\Delta \boldsymbol{Y}_{1|k,m} \in \Re^{km \times N}$.

$$\boldsymbol{U}_{1|k,s} = \begin{bmatrix} \boldsymbol{u}_s(1) & \boldsymbol{u}_s(2) & \cdots & \boldsymbol{u}_s(N) \\ \boldsymbol{u}_s(2) & \boldsymbol{u}_s(3) & \cdots & \boldsymbol{u}_s(N+1) \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{u}_s(k) & \boldsymbol{u}_s(k+1) & \cdots & \boldsymbol{u}_s(N+k-1) \end{bmatrix} \tag{13}$$

$$\Delta \boldsymbol{Y}_{1|k,m} = \begin{bmatrix} \Delta \boldsymbol{y}_m(1) & \Delta \boldsymbol{y}_m(2) & \cdots & \Delta \boldsymbol{y}_m(N) \\ \Delta \boldsymbol{y}_m(2) & \Delta \boldsymbol{y}_m(3) & \cdots & \Delta \boldsymbol{y}_m(N+1) \\ \vdots & \vdots & \ddots & \vdots \\ \Delta \boldsymbol{y}_m(k) & \Delta \boldsymbol{y}_m(k+1) & \cdots & \Delta \boldsymbol{y}_m(N+k-1) \end{bmatrix} \tag{14}$$

where k is a parameter and N must be large enough in comparison with km.

These block Hankel matrices satisfy the following equation derived through LQ decomposition.

$$\begin{bmatrix} \boldsymbol{U}_{1|k,s} \\ \Delta \boldsymbol{Y}_{1|k,m} \end{bmatrix} = \begin{bmatrix} \boldsymbol{L}^s_{11} & \\ \boldsymbol{L}^s_{21} & \boldsymbol{L}^s_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{Q}^T_1 \\ \boldsymbol{Q}^T_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{L}^s_{11} \\ \boldsymbol{L}^s_{21} \end{bmatrix} \boldsymbol{Q}^T_1 \tag{15}$$

where $\boldsymbol{L}^s_{ij}$ and $\boldsymbol{Q}_i$ are matrices derived as a result of the LQ decomposition. The equality is always fulfilled under the assumption that $\Delta \boldsymbol{y}_m$ is affected by only $\boldsymbol{u}_s$. By using Eq. (15), $\boldsymbol{u}_s$ can be estimated from $\boldsymbol{L}^s_{11}$ and $\boldsymbol{Q}_1$, both of which can be derived from $\Delta \boldsymbol{Y}_{1|k,m}$.

The matrix $\boldsymbol{Q}_1 \in \Re^{N \times ks}$ can be generated from the orthogonal matrix $\boldsymbol{V}$ that is derived from SVD of the block Hankel matrix $\Delta \boldsymbol{Y}_{1|k,m}$.

$$\Delta \boldsymbol{Y}_{1|k,m} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T \tag{16}$$

$$\boldsymbol{S} = \begin{bmatrix} \mathrm{diag}\left\{\sigma_1, \sigma_2, \cdots, \sigma_{km}\right\} & \boldsymbol{0}_{(km)\times(N-km)} \end{bmatrix} \tag{17}$$

$$\boldsymbol{V} = \begin{bmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \cdots & \boldsymbol{v}_N \end{bmatrix} \tag{18}$$

where the singular values σ_j are in descending order. All row vectors of $\Delta \boldsymbol{Y}_{1|k,m}$ are mean centered and their standard deviations are scaled to be unity. $\boldsymbol{Q}_1$ is generated from $\boldsymbol{V}$ by selecting ks column vectors corresponding to significant (non-zero) singular values.

$$\boldsymbol{Q}_1 = \begin{bmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_{ks} \end{bmatrix} = \begin{bmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \cdots & \boldsymbol{v}_{ks} \end{bmatrix} \tag{19}$$

$$\boldsymbol{q}_i = \begin{bmatrix} q_{1i} & q_{2i} & \cdots & q_{Ni} \end{bmatrix}^T \tag{20}$$

where s is the number of significant singular values, and it is the same as the number of the estimated disturbance variables $\hat{\boldsymbol{u}}_s$.

The next step is to determine the lower triangular matrix $\boldsymbol{L}_{11}^s \in \Re^{ks \times ks}$, but there is no information about $\boldsymbol{L}_{11}^s$. Therefore, $\Delta \boldsymbol{Y}_{1|k,m}$ is used to determine

$\boldsymbol{L}_{11}^{s}$. It is assumed here that

$$\boldsymbol{L}_{11}^{s} = \begin{bmatrix} \boldsymbol{L}_{11} & & & \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22} & & \\ \vdots & \vdots & \ddots & \\ \boldsymbol{L}_{k1} & \boldsymbol{L}_{k2} & \cdots & \boldsymbol{L}_{kk} \end{bmatrix} \tag{21}$$

$$\boldsymbol{L}_{ii} = \mathrm{diag}\left\{\sigma_{s(i-1)+1}, \sigma_{s(i-1)+2}, \cdots, \sigma_{si}\right\} \tag{22}$$

where σ_j is singular values of $\Delta \boldsymbol{Y}_{1|k,m}$. This assumption ensures that the estimated disturbance variables $\hat{\boldsymbol{u}}_s$ are persistently exciting of order k, because $\boldsymbol{L}_{11}^{s}$ is a regular matrix and $\boldsymbol{Q}_1$ has full column rank.

Since only diagonal blocks are assumed in Eqs. (21) and (22), the lower triangular blocks $\boldsymbol{L}_{ij}(i > j)$ need to be determined. For preparation, the block Hankel matrix $\boldsymbol{U}_{1|k,s}$ is rewritten by

$$\begin{aligned} \boldsymbol{U}_{1|k,s} &= \boldsymbol{L}_{11}^{s} \boldsymbol{Q}_1^T \\ &= \begin{bmatrix} \boldsymbol{L}_{11} & & & \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22} & & \\ \vdots & \vdots & \ddots & \\ \boldsymbol{L}_{k1} & \boldsymbol{L}_{k2} & \cdots & \boldsymbol{L}_{kk} \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_{1,1} & \boldsymbol{q}_{2,1} & \cdots & \boldsymbol{q}_{N,1} \\ \boldsymbol{q}_{1,2} & \boldsymbol{q}_{2,2} & \cdots & \boldsymbol{q}_{N,2} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{q}_{1,k} & \boldsymbol{q}_{2,k} & \cdots & \boldsymbol{q}_{N,k} \end{bmatrix} \end{aligned} \tag{23}$$

where

$$\boldsymbol{q}_{i,j} = \begin{bmatrix} q_{i((j-1)s+1)} & q_{i((j-1)s+2)} & \cdots & q_{i(js)} \end{bmatrix}^T \tag{24}$$

Considering the characteristics of block Hankel matrices, the following equations are derived from Eq. (23):

$$\boldsymbol{u}_s(2) = \boldsymbol{L}_{21}\boldsymbol{q}_{1,1} + \boldsymbol{L}_{22}\boldsymbol{q}_{1,2} = \boldsymbol{L}_{11}\boldsymbol{q}_{2,1} \tag{25}$$

$$\boldsymbol{u}_s(3) = \boldsymbol{L}_{21}\boldsymbol{q}_{2,1} + \boldsymbol{L}_{22}\boldsymbol{q}_{2,2} = \boldsymbol{L}_{11}\boldsymbol{q}_{3,1} \tag{26}$$

Similar equations are derived regarding $\boldsymbol{u}_s(t)(t = 2, 3, \cdots, N)$, and they result in

$$\begin{aligned} &\begin{bmatrix} \boldsymbol{L}_{21} & \boldsymbol{L}_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_{1,1} & \boldsymbol{q}_{2,1} & \cdots & \boldsymbol{q}_{N-1,1} \\ \boldsymbol{q}_{1,2} & \boldsymbol{q}_{2,2} & \cdots & \boldsymbol{q}_{N-1,2} \end{bmatrix} \\ &= \boldsymbol{L}_{11} \begin{bmatrix} \boldsymbol{q}_{2,1} & \boldsymbol{q}_{3,1} & \cdots & \boldsymbol{q}_{N,1} \end{bmatrix} \end{aligned} \tag{27}$$

This equation can be rewritten as

$$\begin{aligned} &\boldsymbol{L}_{21} \begin{bmatrix} \boldsymbol{q}_1^T \\ \vdots \\ \boldsymbol{q}_s^T \end{bmatrix} - \boldsymbol{L}_{21} \begin{bmatrix} \tilde{\boldsymbol{q}}_1^T \\ \vdots \\ \tilde{\boldsymbol{q}}_s^T \end{bmatrix} + \boldsymbol{L}_{22} \begin{bmatrix} \boldsymbol{q}_{s+1}^T \\ \vdots \\ \boldsymbol{q}_{2s}^T \end{bmatrix} \\ &- \boldsymbol{L}_{22} \begin{bmatrix} \tilde{\boldsymbol{q}}_{s+1}^T \\ \vdots \\ \tilde{\boldsymbol{q}}_{2s}^T \end{bmatrix} = \boldsymbol{L}_{11} \begin{bmatrix} \boldsymbol{q}_1^T \\ \vdots \\ \boldsymbol{q}_s^T \end{bmatrix} \boldsymbol{\Xi}_1 - \boldsymbol{L}_{11} \begin{bmatrix} \bar{\boldsymbol{q}}_1^T \\ \vdots \\ \bar{\boldsymbol{q}}_s^T \end{bmatrix} \end{aligned} \tag{28}$$

where

$$\tilde{\boldsymbol{q}}_i \equiv \begin{bmatrix} 0 & 0 & \cdots & 0 & q_{Ni} \end{bmatrix}^T \tag{29}$$

$$\bar{\boldsymbol{q}}_i \equiv \begin{bmatrix} 0 & 0 & \cdots & 0 & q_{i1} \end{bmatrix}^T \tag{30}$$

$$\boldsymbol{\Xi}_i \equiv \left[\begin{array}{c|c} \boldsymbol{0}_{i\times(N-i)} & \boldsymbol{I}_i \\ \hline \boldsymbol{I}_{N-i} & \boldsymbol{0}_{(N-i)\times i} \end{array}\right] \tag{31}$$

and $\boldsymbol{I}_i$ denotes a unit matrix. Eq. (28) post-multiplied by $\boldsymbol{Q}_s$ becomes

$$\boldsymbol{L}_{21}\left(\boldsymbol{I}_s - \begin{bmatrix} \tilde{\boldsymbol{q}}_1^T \\ \vdots \\ \tilde{\boldsymbol{q}}_s^T \end{bmatrix}\boldsymbol{Q}_s\right) = \left(\boldsymbol{L}_{22}\begin{bmatrix} \tilde{\boldsymbol{q}}_{s+1}^T \\ \vdots \\ \tilde{\boldsymbol{q}}_{2s}^T \end{bmatrix} + \boldsymbol{L}_{11}\begin{bmatrix} \tilde{\boldsymbol{q}}_1^T \\ \vdots \\ \tilde{\boldsymbol{q}}_s^T \end{bmatrix}\boldsymbol{\Xi}_1 - \boldsymbol{L}_{11}\begin{bmatrix} \bar{\boldsymbol{q}}_1^T \\ \vdots \\ \bar{\boldsymbol{q}}_s^T \end{bmatrix}\right)\boldsymbol{Q}_s \tag{32}$$

where

$$\boldsymbol{Q}_s = \begin{bmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_s \end{bmatrix} \tag{33}$$

In Eq. (32), only the matrix $\boldsymbol{L}_{21}$ is unknown. Thus, $\boldsymbol{L}_{21}$ can be determined by solving Eq. (32). In the same way, a more general equation can be derived.

$$
\begin{aligned}
&\left[\boldsymbol{L}_{i1} \cdots \boldsymbol{L}_{i(i-1)}\right]\left(\boldsymbol{I}_{s(i-1)} - \begin{bmatrix} \tilde{\boldsymbol{q}}_1^T \\ \vdots \\ \tilde{\boldsymbol{q}}_{s(i-1)}^T \end{bmatrix} \boldsymbol{Q}_{s(i-1)}\right) \\
&= \left\{ \boldsymbol{L}_{ii} \begin{bmatrix} \tilde{\boldsymbol{q}}_{s(i-1)+1}^T \\ \vdots \\ \tilde{\boldsymbol{q}}_{si}^T \end{bmatrix} + \left[\boldsymbol{L}_{(i-1)1} \cdots \boldsymbol{L}_{(i-1)(i-1)}\right] \times \right. \\
&\left. \left(\begin{bmatrix} \boldsymbol{q}_1^T \\ \vdots \\ \boldsymbol{q}_{s(i-1)}^T \end{bmatrix} \boldsymbol{\Xi}_1 - \begin{bmatrix} \bar{\boldsymbol{q}}_1^T \\ \vdots \\ \bar{\boldsymbol{q}}_{s(i-1)}^T \end{bmatrix} \right) \right\} \boldsymbol{Q}_{s(i-1)} \qquad (34)
\end{aligned}
$$

By solving Eq. (34) in sequence, $\boldsymbol{L}_{11}^s$ is derived. Finally, the estimated disturbance variables $\hat{\boldsymbol{u}}_s$ are calculated by using $\boldsymbol{Q}_1$ and $\boldsymbol{L}_{11}^s$.

$$
\begin{aligned}
\hat{\boldsymbol{U}}_{1|k,s} &\equiv \begin{bmatrix} \hat{\boldsymbol{u}}_s(1) & \hat{\boldsymbol{u}}_s(2) & \cdots & \hat{\boldsymbol{u}}_s(N) \\ \hat{\boldsymbol{u}}_s(2) & \hat{\boldsymbol{u}}_s(3) & \cdots & \hat{\boldsymbol{u}}_s(N+1) \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\boldsymbol{u}}_s(k) & \hat{\boldsymbol{u}}_s(k+1) & \cdots & \hat{\boldsymbol{u}}_s(N+k-1) \end{bmatrix} \\
&= \boldsymbol{L}_{11}^s \boldsymbol{Q}_1^T \qquad (35)
\end{aligned}
$$

It is possible to derive $\hat{\boldsymbol{u}}_s$, which is sufficiently excited to build a statistical model through SSID, by using sufficiently large k. In addition, $\hat{\boldsymbol{u}}_s$ at $k = 1$ are persistently exciting when $\Delta \boldsymbol{y}_m$ are generated through an ARMA (autoregressive moving-average) process, because the ARMA process is persistently exciting of infinite order. In such a case, $\hat{\boldsymbol{u}}_s$ can be derived directly from $\Delta \boldsymbol{y}_m$ by using principal component analysis (PCA), and $\hat{\boldsymbol{u}}_s$ are the same as principal component scores.

The parameters to determine in this step for estimating unmeasured disturbances are k and s. The parameter k is related to the persistently exciting condition, and it depends on the characteristics of the process and unmeasured disturbances. In practice, it should be larger than the settling time of the process. On the other hand, the parameter s is the number of unmeasured disturbances. In practice, s is unknown a priori and the estimation performance is affected by the selection of s. The influence of unmeasured disturbances cannot be modeled accurately when s is too small, and over-fitting will occur when s is too large. The derivation of $\hat{\boldsymbol{u}}_s$ from $\Delta \boldsymbol{y}_m$ is just like feature extraction or dimensionality reduction through PCA, in which the number of principal components should be determined. The significance of singular values of $\Delta \boldsymbol{Y}_{1|k,m}$ would be a good indicator. Negligible singular values and their corresponding right singular vectors should not be used.

3.3 Identification (2nd stage)

The two-stage SSID-based softsensor is developed by using measured input variables $\boldsymbol{u}_d$ and the estimated disturbance variables $\hat{\boldsymbol{u}}_s$ as inputs in the state space model of the form:

$$\boldsymbol{x}_2(t+1) = \boldsymbol{A}_2\boldsymbol{x}_2(t) + \boldsymbol{B}_2 \begin{bmatrix} \boldsymbol{u}_d(t) \\ \hat{\boldsymbol{u}}_s(t) \end{bmatrix} \tag{36}$$

$$\boldsymbol{y}_q(t) = \boldsymbol{C}_2\boldsymbol{x}_2(t) + \begin{bmatrix} \boldsymbol{0}_{q\times d} & \boldsymbol{D}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_d(t) \\ \hat{\boldsymbol{u}}_s(t) \end{bmatrix} \tag{37}$$

where the subscript 2 denotes the 2nd stage of identification. This state space model is identified through SSID.

The accuracy of the softsensor does not deteriorate even when unmeasured disturbances are significant, because the two-stage SSID-based softsensor can take into account the influence of unmeasured disturbances on the measured output variables $\boldsymbol{y}_m$ and the key variables $\boldsymbol{y}_q$. In addition, the dynamics from $\boldsymbol{u}_d$ to $\boldsymbol{y}_q$ can be modeled accurately, because the estimated disturbance variables $\hat{\boldsymbol{u}}_s$ do not correlate to $\boldsymbol{u}_d$.

3.4 On-line estimation

On-line estimation is executed by the following procedure.

Step 1: Calculate the estimates of the measured output variables at the present time l, $\hat{\boldsymbol{y}}_m(l)$, through the first state space model (Eqs. (10) and (11)).

Step 2: Derive the residual $\Delta\boldsymbol{y}_m(l)$.

Step 3: Generate matrices $\boldsymbol{Q}_{1,new}$ and $\boldsymbol{L}^s_{11,new}$ by using the left singular matrix $\boldsymbol{U}$ (Eq. (16)) of the block Hankel matrix $\Delta\boldsymbol{Y}_{1|k,m}$. First, derive a principal component score matrix $\boldsymbol{T} \in \Re^{w \times ks}$ by multiplying the block Hankel matrix $\Delta \boldsymbol{Y}_l \in \Re^{km \times w}$, which is generated from residuals, by the loading matrix $\boldsymbol{U}_{ks}$.

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{u}_1 \ \boldsymbol{u}_2 \ \cdots \ \boldsymbol{u}_{km} \end{bmatrix} \in \Re^{km \times km} \tag{38}$$

$$\boldsymbol{U}_{ks} \equiv \begin{bmatrix} \boldsymbol{u}_1 \ \boldsymbol{u}_2 \ \cdots \ \boldsymbol{u}_{ks} \end{bmatrix} \in \Re^{km \times ks} \tag{39}$$

$$\Delta \boldsymbol{Y}_l \equiv \begin{bmatrix} \Delta \boldsymbol{y}_m(l-w-k+2) & \cdots & \Delta \boldsymbol{y}_m(l-k+1) \\ \vdots & \vdots & \vdots \\ \Delta \boldsymbol{y}_m(l-w+1) & \cdots & \Delta \boldsymbol{y}_m(l) \end{bmatrix} \tag{40}$$

$$\boldsymbol{T} = \Delta \boldsymbol{Y}_l^T \boldsymbol{U}_{ks} \tag{41}$$

where w is the number of data points used for disturbance estimation. Each row of $\Delta \boldsymbol{Y}_l$ is scaled by the corresponding means and standard deviations of $\Delta \boldsymbol{Y}_{1|k,m}$. Next, define a matrix $\boldsymbol{S}_{new}$, which corresponds to $\boldsymbol{S}$ in the off-line disturbance estimation step, by using the standard deviation s_i of each column of the score matrix $\boldsymbol{T}$.

$$\boldsymbol{S}_{new} = \sqrt{w-1}\,\mathrm{diag}\left\{ s_1, s_2, \cdots, s_{ks} \right\} \tag{42}$$

Then, calculate $\boldsymbol{Q}_{1,new}$ through

$$\boldsymbol{Q}_{1,new} = \boldsymbol{T}\boldsymbol{S}_{new}^{-1} \tag{43}$$

Finally, calculate the matrix $\boldsymbol{L}_{11,new}^{s}$ by using $\boldsymbol{S}_{new}$ and $\boldsymbol{Q}_{1,new}$ in the same way as the off-line disturbance estimation.

Step 4: Derive estimates of unmeasured disturbances $\hat{\boldsymbol{u}}_s(l)$ by using $\boldsymbol{Q}_{1,new}$ and $\boldsymbol{L}_{11,new}^{s}$.

Step 5: Calculate the estimates of the key variables at the present time l, $\hat{\boldsymbol{y}}_q(l)$, through the second state space model (Eqs. (36) and (37)).

Through this procedure, the key variables $\boldsymbol{y}_q$ can be estimated from measured variables $\boldsymbol{y}_m$ and $\boldsymbol{u}_d$.

4 Numerical Example

To demonstrate the superiority of the proposed two-stage SSID method over the conventional method, their performance is evaluated through a numerical example. The performance of the conventional method based on the Kalman filtering technique is limited due to the assumption that innovations are Gaussian white noises and the properties of disturbances stay constant with time. Therefore, in this section, the estimation performance of both the conventional SSID and the two-stage SSID is compared through their applications to the linear system, to which various disturbances are added.

The system is described by Eqs. (8) and (9), where $\boldsymbol{x} \in \Re^7, \boldsymbol{u}_d \in \Re^3, \boldsymbol{u}_s \in \Re^3, \boldsymbol{y}_q \in \Re^3, \boldsymbol{y}_m \in \Re^7, \boldsymbol{w} \in \Re^7$, and $\boldsymbol{v} \in \Re^{10}$. The unmeasured disturbance variables $\boldsymbol{u}_s$ are Gaussian signals in case 1, stepwise signals in case 2, and a combination of random, stepwise, and ramp-wise signals in case 3. The covariances of $\boldsymbol{w}$ and $\boldsymbol{v}$ are assumed to be unknown.

With the conventional method, a state space model was identified via SSID, states were estimated by using the Kalman filter, then unmeasured output variables were estimated. The number of state variables was determined to be 7, and the covariances of noises were tuned by trial and error so that the estimation performance was maximized. In both methods, 1000 data points were used for modeling and other 500 data points were used for validation, and N4SID (numerical algorithms for subspace state space system identification) [19] was used as an algorithm for SSID.

In case 1, where $\boldsymbol{u}_s$ was Gaussian white noises, both the conventional method and the proposed method were able to estimate unmeasured output variables with great accuracy. The estimation results are summarized in Table 1. The estimation accuracy was evaluated by using the correlation coefficient R between measurements and estimates and RMSE (Root Mean Squared Error). In the two-stage SSID, the parameter was set as $k = 15$ by taking into account the process dynamics, the numbers of state variables in the 1st model and the 2nd model were 7 and 6, respectively, and the number of estimated disturbance variables was 3. These parameters were determined by trial and error. The estimation performance of the conventional SSID method was slightly better than the two-stage SSID method, because innovations were Gaussian white noises and the properties of disturbances stayed constant with time in this case. Thus, the assumption of the Kalman filtering technique was satisfied and the conventional SSID method formed an optimal estimation.

In case 2, where $\boldsymbol{u}_s$ was changed stepwise as shown in Fig. 1, the number of state variables in the conventional SSID method was 8. In the two-stage SSID method, on the other hand, the number of state variables in the 1st model and the 2nd model was 6, the number of estimated disturbance variables was 3, and the parameter $k = 15$. The estimation results are summarized in Table 1 and Fig. 2. The results clearly demonstrate the superiority of the proposed two-stage SSID method over the conventional SSID method.

In case 3, $\boldsymbol{u}_s$ was a combination of random, stepwise, and ramp-wise signals as shown in Fig. 3. The models were the same as those in case 2. That is, the softsensors were developed by using operation data, in which unmeasured disturbances were changed stepwise. The estimation results are summarized in Table 1 and Fig. 4. In addition, the estimated unmeasured disturbances $\hat{\boldsymbol{u}}_s$ are shown in Fig. 5. The two-stage SSID method can outperform the conventional SSID method significantly in estimation performance. In a real production process, various disturbances enter the process and their characteristics change with time. Therefore, the proposed two-stage SSID method will be extremely useful for developing a softsensor.

5 Industrial Case Study

In this section, the usefulness of the proposed two-stage SSID-based softsensor is demonstrated through its application to an industrial ethylene fractionator at Showa Denko K.K. in Japan.

5.1 Ethylene fractionator

A schematic diagram of the industrial ethylene fractionator is shown in Fig. 6. This ethylene fractionator consists of two columns: the bottom column T431 and the top column T432. The feed stream enters the bottom column, and the product ethylene is drawn from the top column. The main specification is the ethane concentration in the ethylene product (16). This fractionator is controlled by multivariable model predictive control. The number of controlled variables, manipulated variables, and disturbance variables is seven, four, and three, respectively. The controlled variables are the ethane concentration and methane concentration in the ethylene product, T431 tray #29 temperature (1), T431 differential pressure, T342 differential pressure, condenser pot level, and reboiler pot level. Manipulated variables are the T431 reboiler flow rate (7), T432 internal reflux flow rate (9), T432 purge flow rate (10), and T432 top pressure (12). The disturbance variables are the T431 feed flow rate, T431 feed ethane concentration (13), and C351 #4 suction pressure (14). Here, C351 is a propylene refrigerant. Its #4 suction pressure affects propylene refrigerant temperature and reboiler heat duty. The numbers in parentheses correspond to those shown in Fig. 6 and Table 2.

5.2 Softsensor Design

Softsensor design is one of the key technologies for reducing off-specification products and enhancing productivity when on-line analyzers are not available. In this study, softsensors that estimate the ethane concentration in the ethylene product are developed through dynamic PLS, SSID, and two-stage SSID.

For building softsensors, operation data obtained from January 1 to February 20, 2002 were used. All variables used for modeling are listed in Table 2. Variables #7, 9, 10, and 12 are classified into manipulated variables $\boldsymbol{u}_{mv}$, variables #8, 11, 13, and 14 are classified into other measured input variables $\boldsymbol{u}_d$, variables #1, 2, 3, 4, 5, 6, and 15 are classified into measured output variables $\boldsymbol{y}_m$, and variable #16 is the key quality variable $\boldsymbol{y}_q$ to estimate.

5.2.1 Dynamic PLS

Kano et al. [4], who investigated steady-state, static, and dynamic PLS-based inferential models, found that the estimation accuracy could be greatly improved by using dynamic PLS (DPLS) models. In addition, Kamohara et al. [13] applied a DPLS-based softsensor to an industrial distillation process, which was investigated in the present work. Therefore, DPLS is used here for developing a softsensor.

All variables listed in Table 2 were used for DPLS modeling. In addition, the operation data including current measurements and those 5, 10, 15, 20, 25, 30, 35, 40, 45 minutes before were used to build a softsensor. The number of latent variables was adjusted to 20. Here, all input variables and an output variable were mean-centered and their standard deviations were scaled to be unity.

5.2.2 Conventional SSID

The advantage of using SSID for softsensor design is that the dynamics of a multivariable process can be easily taken into account, whereas the number of input variables drastically increases in a dynamic PLS approach and input variables should be appropriately selected to achieve the good prediction performance.

In the present work, two types of softsensors were built through conventional SSID to evaluate the effect of using the measured input variables $\boldsymbol{u}_d$ on the estimation accuracy.

- softsensor C1 : $[\boldsymbol{u}_{mv}] \rightarrow [\boldsymbol{y}_q, \boldsymbol{y}_m]$

- softsensor C2 : $[\boldsymbol{u}_{mv}, \boldsymbol{u}_d] \to [\boldsymbol{y}_q, \boldsymbol{y}_m]$

Here, '$[\boldsymbol{a}] \to [\boldsymbol{b}]$' represents a state space model from $\boldsymbol{a}$ to $\boldsymbol{b}$. To identify state space models, N4SID was used. The number of state variables $\boldsymbol{x}$ in C1 and C2 was determined to be 15 on the basis of the estimation results for the validation data. All input and output variables were mean-centered and their standard deviations were scaled to be unity.

5.2.3 Two-stage SSID

In the same way as conventional SSID, two types of softsensors were built through two-stage SSID.

- softsensor TS1

  the first model : $[\boldsymbol{u}_{mv}] \to [\boldsymbol{y}_m]$

  the second model : $[\boldsymbol{u}_{mv}, \hat{\boldsymbol{u}}_s] \to [\boldsymbol{y}_q]$

- softsensor TS2

  the first model : $[\boldsymbol{u}_{mv}, \boldsymbol{u}_d] \to [\boldsymbol{y}_m]$

  the second model : $[\boldsymbol{u}_{mv}, \boldsymbol{u}_d, \hat{\boldsymbol{u}}_s] \to [\boldsymbol{y}_q]$.

To identify state space models, N4SID was used. The results of the past research show that the settling time of this ethylene fractionator is about 50 minutes [13]. Consequently, the value of k is set to 10. The number of estimated disturbance variables $\hat{\boldsymbol{u}}_s$ and the number of state variables $\boldsymbol{x}$ were determined as shown in Table 3. The number of variables was selected by trial and error. All input and output variables were mean-centered and their standard deviations were scaled to be unity.

5.3 Estimation results

The developed softsensors were validated by using operation data obtained from the industrial ethylene fractionator from (a) December 9 through December 16, 2001 and (b) December 21 through December 31, 2001.

The estimation results are shown in Table 4. Here, measurements and estimates of ethane concentration in the ethylene product (Ethane conc.) are scaled. The estimation accuracy of the softsensors was evaluated by both R and RMSE.

In periods (a) and (b), the softsensors C2 and TS2, both of which use $\boldsymbol{u}_d$ as input variables, function better than the others. In addition, the softsensors TS1 and TS2, both of which use $\hat{\boldsymbol{u}}_s$ as input variables, function better than the softsensors C1 and C2, respectively. The results show that the use of measured input variables $\boldsymbol{u}_d$ and estimated unmeasured disturbance variables $\hat{\boldsymbol{u}}_s$ is effective for improving the estimation accuracy of softsensors. In the same period, the DPLS-based softsensor shows better estimation accuracy than the softsensors C1 and TS1, both of which do not use $\boldsymbol{u}_d$ as input variables. In conclusion of this industrial case study, the proposed two-stage subspace identification (SSID) was confirmed to be effective in designing softsensors.

6 Conclusions

In the present work, two-stage subspace identification (SSID) was proposed to develop an accurate softsensor that could take into account the influence of unmeasured disturbances on estimated key variables such as product quality.

The two-stage SSID procedure is as follows: 1) identify a state space model by using measured input and output variables, 2) estimate unmeasured disturbance variables from residual variables, and 3) identify a state space model to estimate key variables from the estimated disturbance variables and the other measured input variables. The proposed two-stage SSID can estimate unmeasured disturbances without assumptions that the conventional Kalman filtering technique must make. Thus it can outperform the Kalman filtering technique when innovations are not Gaussian white noises or the properties of disturbances do not stay constant with time. The superiority of the proposed method over the conventional methods, i.e., dynamic PLS and SSID, was demonstrated on an industrial ethylene fractionator. It is expected that the two-stage SSID will function successfully in various industrial processes.

Acknowledgements

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References

[1] M. Kano, Y. Nakagawa, Data-based process monitoring, process control, and quality improvement: recent developments and applications in steel industry, Computers & Chemical Engineering 32 (2008) 12–24.

[2] T. Mejdell, S. Skogestad, Estimation of distillation compositions from multiple temperature measurements using partial-least-squares regression, Industrial & Engineering Chemistry Research 30 (1991) 2543–2555.

[3] J. V. Kresta, T. E. Marlin, J. F. MacGregor, Development of inferential process models using PLS, Computers & Chemical Engineering 18 (1994) 597–611.

[4] M. Kano, K. Miyazaki, S. Hasebe, I. Hashimoto, Inferential control system of distillation compositions using dynamic partial least squares regression, Journal of Process Control 10 (2000) 157–166.

[5] B. Lin, B. Recke, J. K. H. Knudsen, S. B. Jorgensen, A systematic approach for soft sensor development, Computers & Chemical Engineering 31 (2007) 419–425.

[6] P. Nomikos, J. F. MacGregor, Multiway Partial Least Squares in Monitoring Batch Processes, Chemometrics and Intelligent Laboratory Systems 30 (1995) 97–109.

[7] J. Flores-Cerrillo, J. F. MacGregor, Within-batch and batch-to-batch inferential-adaptive control of semibatch reactors: A partial least squares approach, Industrial & Engineering Chemistry Research 42 (2003) 3334–3345.

[8] J. Flores-Cerrillo, J. F. MacGregor, Control of batch product quality by trajectory manipulation using latent variable models, Journal of Process Control 14 (2004) 539–553.

[9] D. Aguado, A. Ferrer, A. Seco, J. Ferrer, Comparison of different predictive models for nutrient estimation in a sequencing batch reactor for wastewater treatment, Chemometrics and Intelligent Laboratory Systems 84 (2006) 75–81.

[10] N. Y. Lu, Y. Yang, F. R. Gao, F. L. Wang, Multirate dynamic inferential modeling for multivariable processes, Chemical Engineering Science 59 (2004) 855–864.

[11] S. J. Qin, Recursive PLS algorithms for adaptive data modeling, Computers & Chemical Engineering 22 (1998) 503–514.

[12] S. J. Mu, Y. Z. Zeng, R. L. Liu, P. Wu, H. Y. Su, J. Chu, Online dual updating with recursive PLS model and its application in predicting crystal size of purified terephthalic acid (PTA) process, Journal of Process Control 16 (2006) 557–566.

[13] H. Kamohara, A. Takinami, M. Takeda, M. Kano, S. Hasebe, I. Hashimoto, Product quality estimation and operating condition monitoring for industrial ethylene fractionator, Journal of Chemical Engineering of Japan 37 (2004) 422–428.

[14] R. Amirthalingam, J. H. Lee, Subspace identification based inferential control applied to a continuous pulp digester, Journal of Process Control 9 (1999) 397–406.

[15] R. Amirthalingam, S. W. Sung, J. H. Lee, Two-step procedure for data-based modeling for inferential control applications, AIChE Journal 46 (2000) 1974–1988.

[16] A. W. Dorsey, J. H. Lee, Building inferential prediction models of batch processes using subspace identification, Journal of Process Control 13 (2003) 397–406.

[17] J. H. Lee, A. W. Dorsey, Monitoring of batch processes through state-space models, AIChE Journal 50 (2004) 1198–1210.

[18] T. Katayama, Subspace methods for system identification, Asakura, Tokyo, 2004.

[19] P. V. Overschee, B. D. Moor, N4SID: Subspace algorithms for the identification of combined deterministic-stochastic systems, Automatica 30 (1994) 75–93.

Figure Captions

Fig. 1 Unmeasured disturbance $\boldsymbol{u}_s$ for modeling in case 2.

Fig. 2 Estimation results through conventional SSID and two-stage SSID in case 3. (solid line: measurements, dotted line: estimates with conventional SSID, gray line: estimates with two-stage SSID)

Fig. 3 Unmeasured disturbance $\boldsymbol{u}_s$ for validation in case 3.

Fig. 4 Estimation results through conventional SSID and two-stage SSID in case 3. (solid line: measurements, dotted line: estimates with conventional SSID, gray line: estimates with two-stage SSID)

Fig. 5 Estimated unmeasured disturbance $\hat{\boldsymbol{u}}_s$ in case 3.

Fig. 6 Schematic diagram of the industrial ethylene fractionator T431/2 (C351 is a propylene compressor. Propylene is used for heating or cooling at the reboiler and the condensor.)

Fig. 7 Estimation results of the ethane concentration in the ethylene product by using DPLS, SSID (C1 and C2), and two-stage SSID (TS1 and TS2). (solid line: measurements, dotted line: estimates)

Fig. 8 Time series data of the industrial ethylene fractionator. Key variable to estimate (top), one of manipulated variables (middle), and one of estimated unmeasured disturbances (bottom).

Table 1

Comparison of the estimation performance of softsensor design methods.

	Conv-SSID			TS-SSID		
	$y_{q,1}$	$y_{q,2}$	$y_{q,3}$	$y_{q,1}$	$y_{q,2}$	$y_{q,3}$
Case 1						
R	0.96	0.98	0.95	0.95	0.92	0.95
RMSE	8.32	3.58	15.85	9.01	7.67	16.51
Case 2						
R	0.90	0.96	0.96	0.96	0.96	0.94
RMSE	28.52	17.41	69.10	16.00	9.08	28.86
Case 3						
R	0.38	0.88	0.47	0.97	0.92	0.94
RMSE	62.59	14.19	98.11	17.77	12.07	38.43

Table 2

Variables used for modeling

No.	Variable
1	T431 tray #29 temperature
2	T431 bottom temperature
3	T431 top temperature
4	T431 tray #37 temperature
5	T431 tray #129 temperature
6	Flow rate from T432 to T431
7	T431 reboiler flow rate
8	Product ethylene flow rate
9	T432 internal reflux flow rate
10	T432 purge flow rate
11	T432 reflux ratio
12	T432 top pressure
13	T431 feed ethane concentration
14	C351 #4 suction pressure
15	V359 level (cooling propylene)
16	Ethane concentration in the ethylene product

Table 3

The number of variables used in two-stage SSID

		TS1	TS2
State variables $\boldsymbol{x}$	First model	5	10
	Second model	6	6
Estimated disturbance variables $\hat{\boldsymbol{u}}_s$		5	4

Table 4

Comparison of softsensors developed through DPLS, SSID (C1 and C2), and two-stage SSID (TS1 and TS2) by using validation data sets (a) December 9 through December 16, 2001 and (b) December 21 through December 31, 2001.

	R		RMSE	
	(a)	(b)	(a)	(b)
DPLS	0.75	0.74	5.34	4.18
Conventional SSID				
C1	0.13	0.39	9.86	6.72
C2	0.88	0.85	6.79	3.69
Two-stage SSID				
TS1	0.70	0.54	9.64	6.30
TS2	0.90	0.88	4.28	2.97

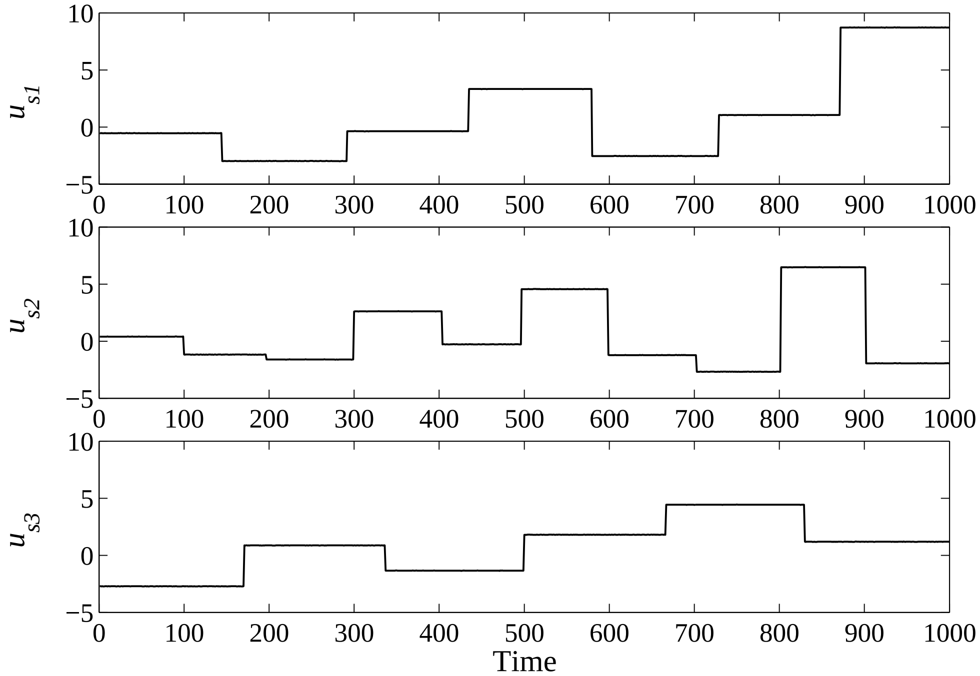

Fig. 1. Unmeasured disturbance $\boldsymbol{u}_s$ for modeling in case 2.

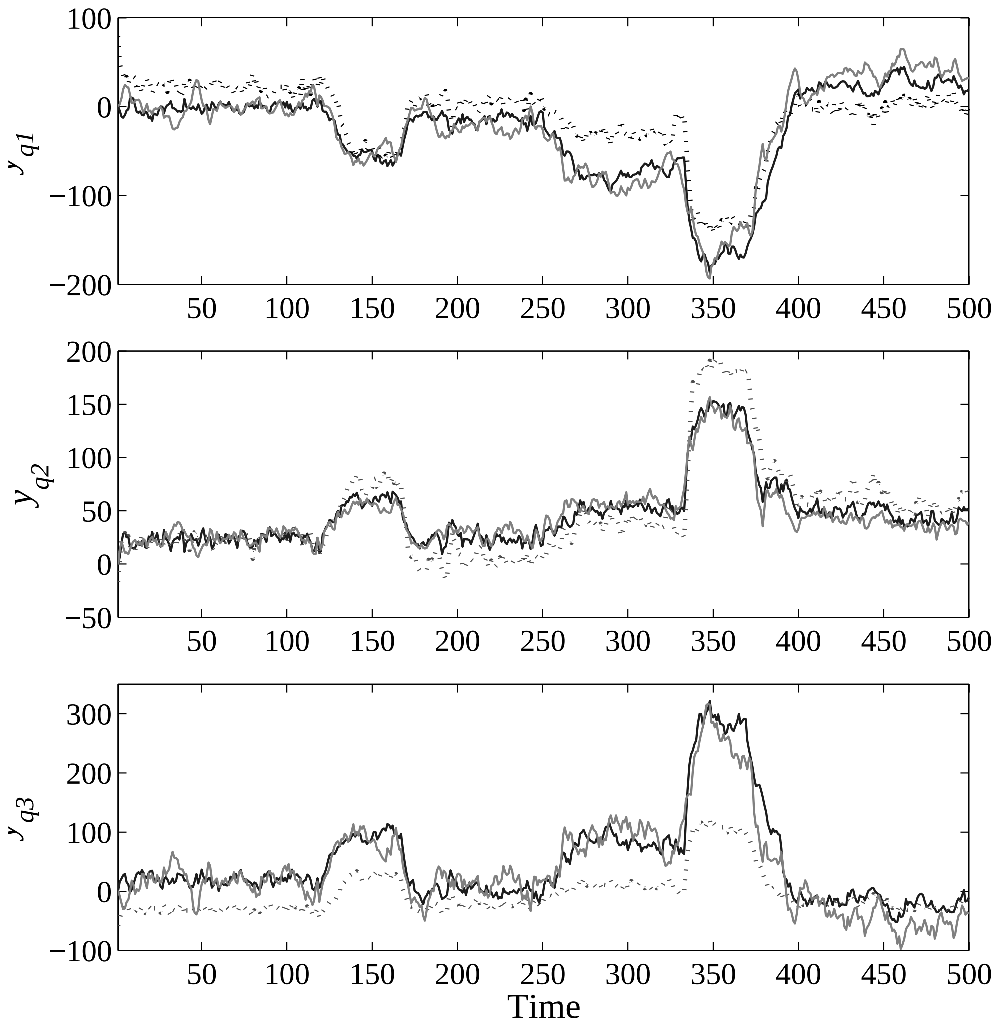

Fig. 2. Estimation results through conventional SSID and two-stage SSID in case 3. (solid line: measurements, dotted line: estimates with conventional SSID, gray line: estimates with two-stage SSID)

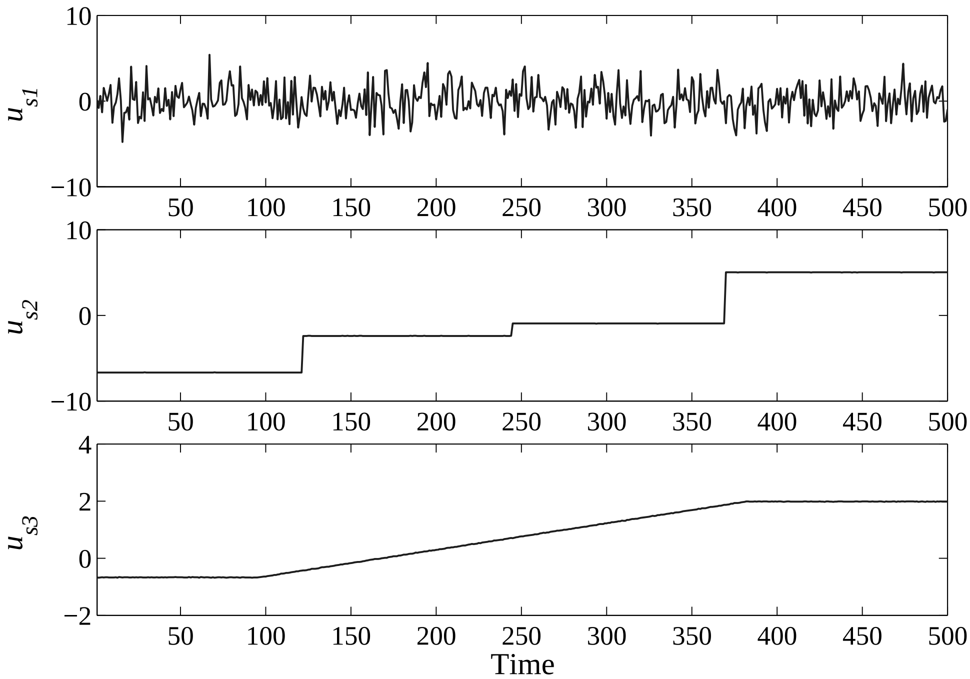

Fig. 3. Unmeasured disturbance $\boldsymbol{u}_s$ for validation in case 3.

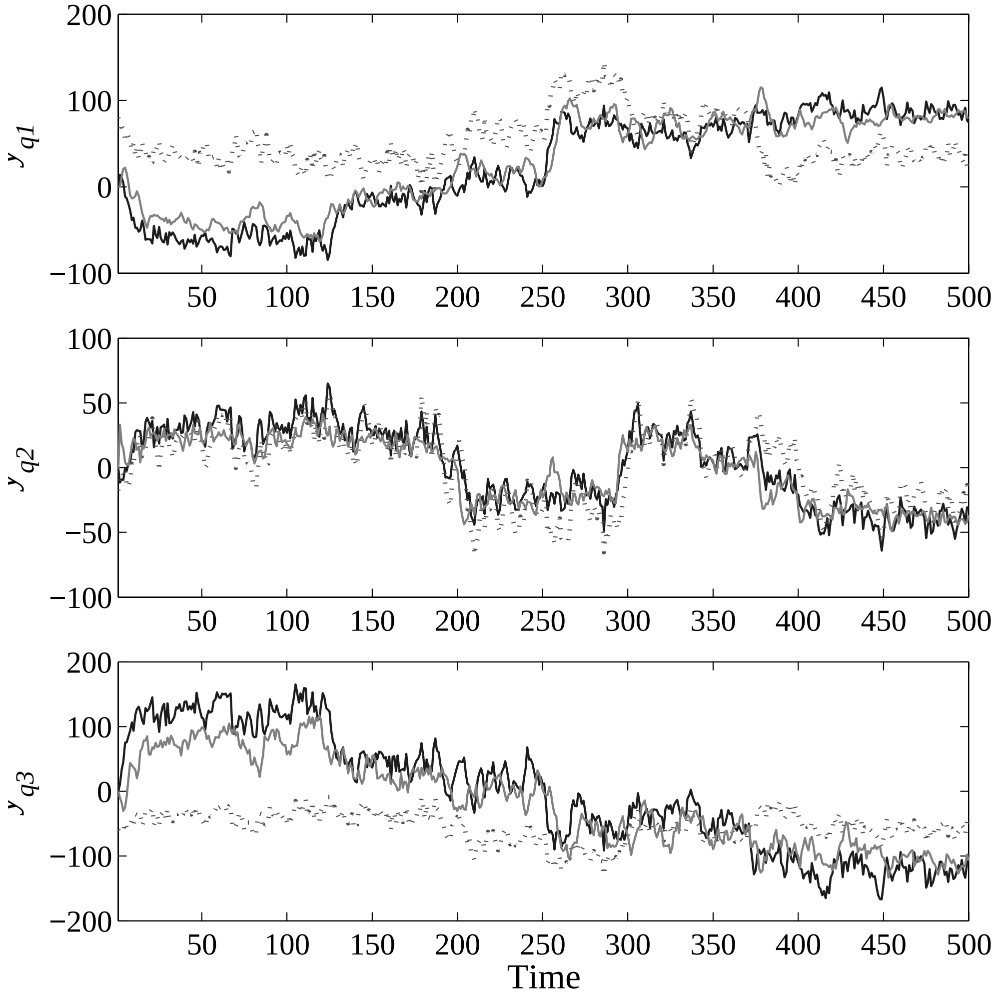

Fig. 4. Estimation results through conventional SSID and two-stage SSID in case 3. (solid line: measurements, dotted line: estimates with conventional SSID, gray line: estimates with two-stage SSID)

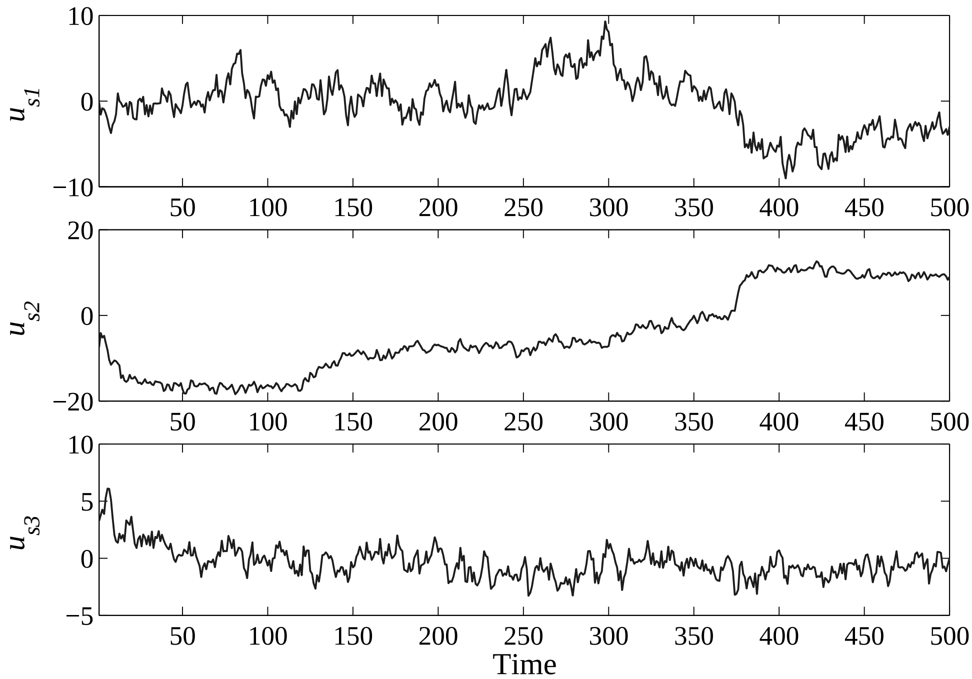

Fig. 5. Estimated unmeasured disturbance $\hat{\boldsymbol{u}}_s$ in case 3.

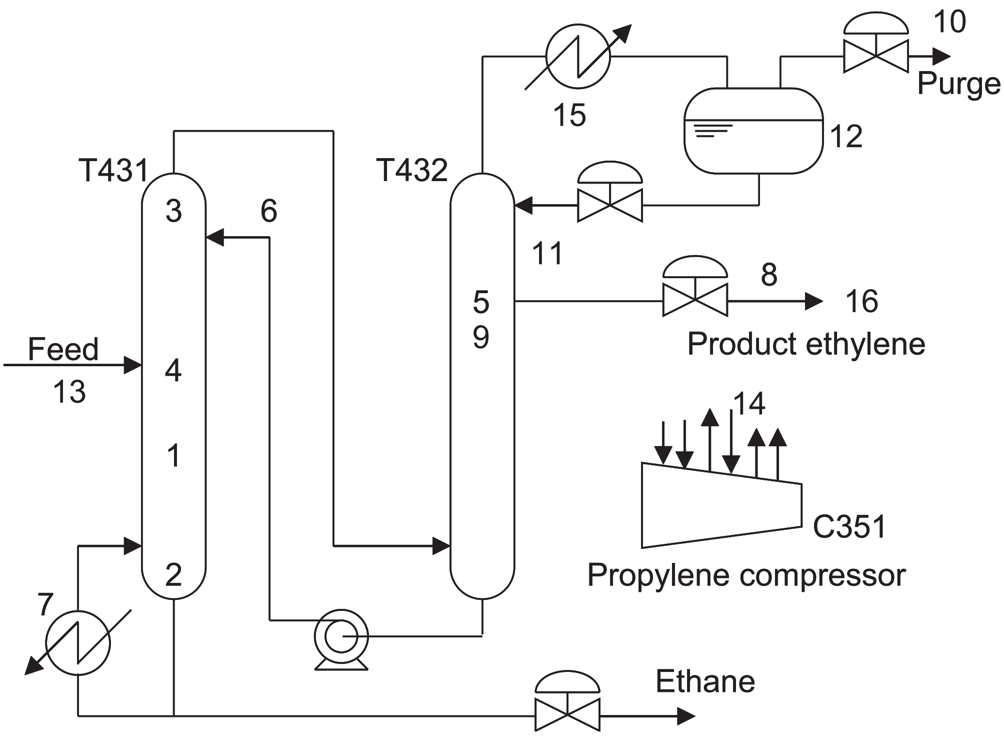

Fig. 6. Schematic diagram of the industrial ethylene fractionator T431/2 (C351 is a propylene compressor. Propylene is used for heating or cooling at the reboiler and the condensor.)